Surrogate Modeling and Parameter Estimation Exercise

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Wednesday, March 25th, 2025

Exercise Overview

- **Objective:** Build a surrogate model for an expensive analytical function and use it to estimate the optimal parameter.
- **Tasks:**
  1. Construct a surrogate for a misfit function.
  2. Find the local optimum of the surrogate to determine the parameter that best fits the data.

The Expensive Model

- We consider the following analytical model:

$$f(\theta) = (\theta - 2)^2 + 0.5 \sin(5\theta)$$

- **Interpretation:** This function represents an expensive-to-evaluate process parameterized by θ.

Hypothetical Observation and Misfit Function

- **Observation:** We assume a hypothetical observation:

$$y_{\text{obs}} = 1.0$$

- **Misfit Function:** The misfit (or loss) function is defined as:

$$J(\theta) = \left(f(\theta) - y_{\text{obs}}\right)^2$$

- **Goal:** Find the parameter θ that minimizes $J(\theta)$.

Surrogate Modeling Concept

- **Challenge:** Evaluating the expensive model $f(\theta)$ and the misfit $J(\theta)$ can be computationally demanding.
- **Idea:** Build a *surrogate model* that approximates the misfit function using data sampled over the domain.
- **Example:** Use polynomial regression (e.g., degree 4) to fit a surrogate function $\tilde{J}(\theta)$ based on sample points.

Surrogate Model Construction

- **Step 1: Sampling** Generate a set of sample points:

$$\theta \in [0, 4]$$

  and compute the corresponding misfit values $J(\theta)$.
- **Step 2: Regression** Fit a polynomial (e.g., using least-squares) to obtain coefficients for $\tilde{J}(\theta)$.
- **Benefit:** The surrogate $\tilde{J}(\theta)$ is much cheaper to evaluate and differentiable.

Surrogate Optimization

- Use a local optimization method (e.g., a gradient-based optimizer) on the surrogate $\tilde{J}(\theta)$.
- **Objective:** Find θ_{opt} such that:

$$\theta_{\text{opt}} = \underset{\theta}{\operatorname{argmin}}\, \tilde{J}(\theta)$$

- **Comparison:** For validation, compare the surrogate optimum with a grid search on the true misfit $J(\theta)$.

Summary and Discussion

- We used an analytical function with parameter θ:

$$f(\theta) = (\theta - 2)^2 + 0.5\sin(5\theta)$$

- With a hypothetical observation $y_{\text{obs}} = 1.0$, we defined the misfit function:

$$J(\theta) = \left(f(\theta) - y_{\text{obs}}\right)^2$$

- A surrogate model $\tilde{J}(\theta)$ is built to approximate $J(\theta)$ based on sample data.
- Finally, a local optimizer is applied to the surrogate model to determine the optimal parameter, which is then compared with the true misfit.

Next Steps

- **Implementation:** Complete the Python code to fit the surrogate model and run the optimization.
- **Extensions:**
  - Experiment with different surrogate models (e.g., Gaussian processes, neural networks).
  - Analyze the impact of sample size and polynomial degree on the optimization accuracy.

Conclusion

- Surrogate modeling provides an efficient way to approximate expensive functions.
- It enables effective parameter estimation by reducing computational cost.
- This exercise lays the foundation for further exploration in surrogate-assisted optimization and uncertainty quantification.